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COMPUTATION OF GENERAL TOPOLOGICAL INDICES FOR TITANIA NANOTUBES

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ABSTRACT

A single number that can be used to characterize some property of the graph of a molecular is called a topological index for that graph. The concepts of generalized version of the first zegeb index, general connectivity index, general sum connectivity index, general reformulated index were established in chemical graph theory based on vertex degrees. In this paper, we compute generalized version of the first zagrab index, general connectivity index, general sum connectivity index, general reformulated index, and other connectivity indices for titania nanotubes.

Keywords: *First Zagreb index, connectivity index, sum connectivity index, reformulated index, K-edge index, titania nanotube.*

AMS Subject Classification: *05C05,*

1. INTRODUCTION

Let G be a finite, simple and connected graph with a vertex set $V(G)$ and an edge set $E(G)$. The degree $d_G(v)$ of a vertex v is the number of vertices adjacent to v. The degree of an edge $e = uv$ in G is defined by $d_G(e) = d_G(u) + d_G(v) – 2$. For all further notation and terminology we refer to reader to [1].

A molecular graph is a graph such that its vertices correspond to the atoms and the edges to the bonds. Chemical graph theory is a branch of mathematical chemistry which has an important effect on the development of the chemical sciences. A single number that can be used to characterize some property of the graph of a molecular is called a topological index for that graph. There are several topological descriptors that have some applications in theoretical chemistry, especially in QSPR/QSAR research.

In [2], the first and second Zegreb indices were introduced by Gutman *et al.* in 1972 and it was stated that these indices are useful in a study of certain chemicals. They are respectively defined as

$$M_1(G) = \sum_{u \in V(G)} d_G(u)^2 \qquad \text{or} \qquad M_1(G) = \sum_{uv \in E(G)} \left[d_G(u) + d_G(v)\right].$$

$$M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v).$$

In [3], Li et al. introduced the generalized version of the first Zagreb index, and it is defined as

$$M_1^{a+1}(G) = \sum_{u \in V(G)} d_G(u)^{a+1} = \sum_{uv \in E(G)} \left[d_G(u)^a + d_G(v)^a\right], \quad \text{where } a \in R. \tag{1}$$

The modified first and second Zagreb indices [4] are respectively defined as

$$^{m}M_1(G) = \sum_{u \in V(G)} \frac{1}{d_G(u)^2}, \qquad ^{m}M_2(G) = \sum_{uv \in E(G)} \frac{1}{d_G(u) d_G(v)}.$$

The F-index of a graph G is defined as

$$F(G) = \sum_{u \in V(G)} d_G(u)^3.$$

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This index was introduced in [2]. In [5], Furtula and Gutman studied this index and called it forgotten topological index.

In [6], Shirdel *et al.* introduced the first hyper-Zagreb index of a graph *G*, which is defined as

$$HM_1(G) = \sum_{uv \in E(G)} \left[d_G(u) + d_G(v) \right]^2.$$

In [7], Zhou and Trinajstić introduced the sum connectivity index of a graph *G* which is defined as

$$X(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u) + d_G(v)}}.$$

The general sum connectivity index was introduced by Zhou and Trinajstić in [8] and it is defined as

$$M_1^a(G) = \sum_{uv \in E(G)} \left[d_G(u) + d_G(v) \right]^a. \tag{2}$$

This index was studied, for example, in [9].

In [10], the second hyper-Zagreb index of a graph *G* is defined as

$$HM_2(G) = \sum_{uv \in E(G)} \left[d_G(u) d_G(v) \right]^2.$$

The Randić index or product connectivity index of a graph *G* is defined as

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u) d_G(v)}}.$$

This topological index was proposed by Randić in [11] and was studied, for example in [12, 13].

The general Randić index [9, 14] is defined as

$$M_2^a(G) = \sum_{uv \in E(G)} \left[d_G(u) d_G(v) \right]^a. \tag{3}$$

The reformulated first Zagreb index of a graph *G* is defined as

$$EM_1(G) = \sum_{e \in E(G)} d(e)^2.$$

This index was introduced by Miličević *et al.* in [15].

Very recently in [16], Kulli introduced the *K*-edge index of a graph *G* and it is defined as

$$K_e(G) = \sum_{e \in E(G)} d(e)^3.$$

This index was also studied in [17].

The general reformulated Zagreb index of a graph *G* is defined as

$$EM_1^a(G) = \sum_{e \in E(G)} d(e)^{a+1}, \tag{4}$$

where *a* is a real number.

In this paper, we determine several topological indices for titania nanotubes $TiO_2[m, n]$.

2. RESULTS FOR TiO_2 NANOTUBES

Titania is studied in materials science. The titania nanotubes usually symbolized as $TiO_2[m, n]$ for $m, n \in N$, in which *m* is the number of octagons C_8 in a row and *n* is the number of octagons C_8 in a column. The graph of $TiO_2[m, n]$ is shown in Figure 1.

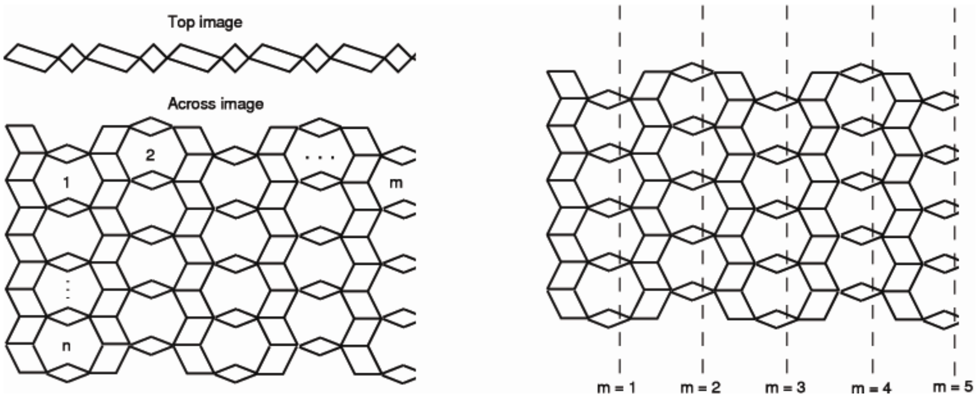

Figure-1: The graph of TiO_2[m, n]-nanotubes with m = 5 and n = 4.

By algebraic method, we obtains $|V(TiO_2[m, n])| = 6n(m+1)$. From Figure 1, it is easy to see that there are four partitions of the vertex set of TiO_2 as follows:

Let $G = TiO_2[m,n]$.

$V_2 = \{u\in V(G) \mid d_G(u) = 2\}, |V_2| = 2mn + 4n.$

$V_3 = \{u\in V(G) \mid d_G(u) = 3\}, |V_3| = 2mn.$

$V_4 = \{u\in V(G) \mid d_G(u) = 4\}, |V_4| = 2n.$

$V_5 = \{u\in V(G) \mid d_G(u) = 5\}, |V_5| = 2mn.$

Also, by algebraic method, we obtain three edge partitions of G based on the sum of degrees of the end vertices as follows:

$E_6 = \{uv\in E(G) \mid d_G(u) = 2, d_G(v) = 4\}, \quad |E_6| = 6n.$

$E_7 = \{uv\in E(G) \mid d_G(u) = 2, d_G(v) = 5\}\cup\{uv\in E(G) \mid d_G(u) = 3, d_G(v) = 4\}, \ |E_7| = 4mn + 4n.$

$E_8 = \{uv\in E(G) \mid d_G(u) = 3, d_G(v) = 5\}, \quad |E_8| = 6mn - 2n.$

Similarly, by algebraic method, we obtain four edge partitions of G based on the product of degrees of the end vertices as follows:

$$E_8^* = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 4\}, \ |E_8^*| = 6n.$$

$$E_{10}^* = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 5\}, \ |E_{10}^*| = 4mn + 2n.$$

$$E_{12}^* = \{uv \in E(G) \mid d_G(u) = 3, d_G(v) = 4\}, \ |E_{12}^*| = 2n.$$

$$E_{15}^* = \{uv \in E(G) \mid d_G(u) = 3, d_G(v) = 5\}, \ |E_{15}^*| = 6mn - 2n.$$

The edge degree partition of G is given in Table 1.

$d_G(u), d_G(v) \setminus e=uv \in E(G)$	$E_6 = (2, 4)$	$E_7 = (2, 5) \cup (3, 4)$	$E_8 = (3, 5)$
$d_G(e)$	4	5	6
Number of edges	$6n$	$4mn + 4n$	$6mn - 2n$

Table-1: Edge degree partition of TiO_2

In the following theorem, we determine the generalized version of the first Zagreb index of the TiO_2 nanotube.

Theorem 1: The generalized version of the first Zagreb index of TiO_2 nanotube is given by

$$M_1^{a+1}(TiO_2) = \left(2^{a+1} + 3^{a+1} + 5^{a+1}\right)2mn + \left(4\times 2^{a+1} + 2\times 4^{a+1}\right)n. \tag{5}$$

Proof: Let $G = TiO_2\ [m, n]$. From equation (1) and by cardinalities of the vertex partitions of TiO_2 nanotube, we have

$$M_1^{a+1}(G) = \sum_{u\in V(G)} d_G(u)^{a+1} = \sum_{u\in V_2} d_G(u)^{a+1} + \sum_{u\in V_3} d_G(u)^{a+1} + \sum_{u\in V_4} d_G(u)^{a+1} + \sum_{u\in V_5} d_G(u)^{a+1}$$

$$= 2^{a+1}(2mn + 4n) + 3^{a+1}(2mn) + 4^{a+1}(2n) + 5^{a+1}(2mn)$$

$$= \left(2^{a+1} + 3^{a+1} + 5^{a+1}\right)2mn + \left(4\times 2^{a+1} + 2\times 4^{a+1}\right)n.$$

An immediate corollary is the first Zagreb index of TiO_2 nanotube.

Corollary 1.1: The first Zagrab index of TiO_2 nanotube is given by

$$M_1(TiO_2) = 76mn + 48n.$$

Proof: Put $a = 1$ in equation (5), we get the desired result.

An immediate another corollary is the F- index of TiO_2 nanotube.

Corollary 1.2: The F- index of TiO_2 nanotube is given by

$$F(TiO_2) = 320mn + 160n.$$

Proof: Put $a = 2$ in equation (5), we get the desired result.

Another corollary is the modified first Zagreb index of TiO_2 nanotube.

Corollary 1.3: The modified first Zagreb index of TiO_2 nanotube is given by

$$^{m}M_1\left(TiO_2\right)=\left(\frac{293}{450}\right)mn+\frac{9}{8}n.$$

Proof: Put $a = -3$ in equation (5), we get the desired result.

We now determine the general sum connectivity index of TiO_2 nanotube.

Theorem 2: The general sum connectivity index of TiO_2 nanotube is given by

$$M_1^a\left(TiO_2\right)=\left(4\times7^a+6\times8^a\right)mn+\left(6\times6^a+4\times7^a-2\times8^a\right)n. \tag{6}$$

Proof: From equation (2) and by cardinalities of the edge partitions of TiO_2 nanotube, we have

$$M_1^a\left(G\right)=\sum_{uv\in E(G)}\left[d_G\left(u\right)+d_G\left(v\right)\right]^a=\sum_{uv\in E_6}\left[d_G\left(u\right)+d_G\left(v\right)\right]^a+\sum_{uv\in E_7}\left[d_G\left(u\right)+d_G\left(v\right)\right]^a+\sum_{uv\in E_8}\left[d_G\left(u\right)+d_G\left(v\right)\right]^a$$

$$=6^a\times6n+7^a\times\left(4mn+4n\right)+8^a\times\left(6mn-2n\right)$$

$$=\left(4\times7^a+6\times8^a\right)mn+\left(6\times6^a+4\times7^a-2\times8^a\right)n.$$

An immediate corollary is the first Zagreb index of TiO_2 nanotube.

Corollary 2.1: The first Zagreb index of TiO_2 nanotube is given by

$$M_1(TiO_2) = 76mn + 48n.$$

Proof: Put $a=1$ in equation (6), we get the desired result.

An immediate another corollary in the hyper Zagreb index of TiO_2 nanotube.

Corollary 2.2: The first hyper Zagreb index of TiO_2 nanotube is given by

$$HM_1(TiO_2) = 580mn + 284n.$$

Proof: Put $a = 2$ in equation (6), we get the desired result.

Next, corollary is the sum connectivity of index of TiO_2 nanotube.

Corollary 2.3: The sum connectivity index of TiO_2 nanotube is given by

$$X\left(G\right)=\left(\frac{4}{\sqrt{7}}+\frac{3}{\sqrt{2}}\right)mn+\left(\frac{6}{\sqrt{6}}+\frac{4}{\sqrt{7}}-\frac{1}{\sqrt{2}}\right)n.$$

Proof: Put $a=-\frac{1}{2}$ in equation (6), we get the desired result.

In the next result, we compute the general Randić index of TiO_2 nanotube.

Theorem 3: The general Randić index of TiO_2 nanotube is given by

$$M_2^a\left(TiO_2\right)=\left(4\times10^a+6\times15^a\right)mn+\left(6\times8^a+2\times10^a+2\times12^a-2\times15^a\right)n. \tag{7}$$

Proof: Let $G = TiO_2$. From equation (3) and by cardinalities of the edge partitions of G based on the product of degrees of the end vertices, we have

$$M_2^{(a)}\left(TiO_2\right) = \sum_{uv\in E(G)} \left[d_G(u).d_G(v)\right]^a$$

$$= \sum_{uv\in E_8^*}\left[d_G(u)d_G(v)\right]^a + \sum_{uv\in E_{10}^*}\left[d_G(u)d_G(v)\right]^a + \sum_{uv\in E_{12}^*}\left[d_G(u)d_G(v)\right]^a + \sum_{uv\in E_{15}^*}\left[d_G(u)d_G(v)\right]^a$$

$$= 8^a \times 6n + 10^a \times \left(4mn + 2n\right) + 12^a \times 2n + 15^a \times \left(6mn - 2n\right)$$

$$= \left(4\times 10^a + 6\times 15^a\right)mn + \left(6\times 8^a + 2\times 10^a + 2\times 12^a - 2\times 15^a\right)n.$$

An immediate corollary is the second Zagreb index of TiO_2 nanotube.

Corollary 3.1: The second Zagreb index of TiO_2 is given by

$$M_2(TiO_2) = 130mn + 62n.$$

Proof: Put $a = 1$ in equation (7), we get the desired result.

An immediate another corollary is the second hyper Zagreb index of TiO_2 nanotube.

Corollary 3.2: The second hyper-Zagreb index of TiO_2 nanotube is given by

$$HM_2(TiO_2) = 1750mn + 422n.$$

Proof: Put $a = 2$ in equation (7), we get the desired result.

Next, corollary is the modified second Zagreb index of TiO_2 nanotube.

Corollary 3.3: The modified second Zagreb index of TiO_2 nanotube is given by

$$^m M_2\left(TiO_2\right) = \frac{4}{5}mn + \frac{59}{60}n.$$

Proof: Put $a = -1$ in equation (7), we get the desired result.

An immediate another corollary is the Randić connectivity index of TiO_2 nanotube.

Corollary 3.4: The Randić connectivity index of TiO_2 nanotube is given by

$$\chi\left(TiO_2\right) = \left(\frac{4}{\sqrt{10}} + \frac{6}{\sqrt{15}}\right)mn + \left(\frac{6}{\sqrt{8}} + \frac{2}{\sqrt{10}} + + \frac{2}{\sqrt{12}} - \frac{2}{\sqrt{15}}\right)n.$$

Proof: Put $a = -\frac{1}{2}$ in equation (7), we get the desired result.

In the following theorem, we determine the general first reformulated Zagreb index of TiO_2 nanotubes.

Theorem 4: The general first reformulated Zagreb index of TiO_2 nanotubes is given by

$$EM_1^a\left(TiO_2\right) = \left(4\times 5^a + 6\times 6^a\right)mn + \left(6\times 4^a + 4\times 5^a - 2\times 6^a\right)n. \tag{8}$$

Proof: Let $G = TiO_2$. From equation (4) and by the edge degree partitions of G, we have

$$EM_1^a\left(TiO_2\right) = \sum_{e\in E(G)} d_G(e)^a = \sum_{e\in E_6} d_G(e)^a + \sum_{e\in E_7} d_G(e)^a + \sum_{e\in E_8} d_G(e)^a$$

$$= 4^a\left(6n\right) + 5^a\left(4mn + 4n\right) + 6^a\left(6mn - 2n\right)$$

$$= \left(4\times 5^a + 6\times 6^a\right)mn + \left(6\times 4^a + 4\times 5^a - 2\times 6^a\right)n.$$

The following results are immediate from Theorem 4.

Corollary 4.1: The first reformulated Zagreb index of TiO_2 nanotube is given by

$$EM_1(TiO_2) = 316\,mn + 124n.$$

Proof: Put $a = 2$ in equation (8), we obtain the desired result.

Corollary 4.2: The K-edge index of TiO_2 nanotube is given by

$$K_e(TiO_2) = 1796mn + 452n.$$

Proof: Put $a = 3$ in equation (8), we obtain the desired result.

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